

DATA EVALUATION RECORD

STUDY 6

CHEM 128976

UNICONAZOLE

163-2

BRANCH EAB

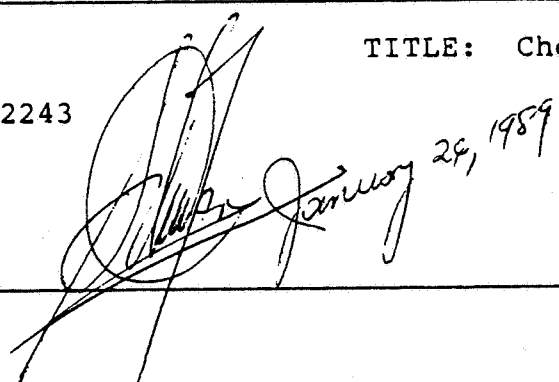
FORMULATION OO-Formulated material with radiolabeled active ingredient

EPA MRID No. 40462604. Katagi, T., Takahashi, N., Mikami, N., Matsuda, T., and Yamada, H. 1987. Volatilization of S-3307D from soil surface. Performed by Sumitomo Chemical Company, Hyogo, Japan. Laboratory Project Identification IIW-70-0016. Completed June 9, 1987. Submitted by Chevron Chemical Company, Richmond, CA.

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CONCLUSIONS:

This study is acceptable and fulfills data requirements for volatilization of uniconazole from soil.

The results (sand soil) showed that during the 30-day period of the experiment, 0.012-0.014% of the applied radioactivity volatilized from the soil. At the end of the test period, ca. 100% of the initial dosage remained in the soil. About 92% of the applied radioactivity was extracted from the soil with methanol/water; the extract consisted primarily of the unchanged parent (S)-(E)-isomer with a trace amount of the Z-isomer. In the extracts from the traps used for trapping volatile materials, the parent compound was also the main component.

Volatilization rate and air concentration were maximal on the first day after treatment, but decreased afterwards. The calculated volatilization rate was  $7.50_3 \times 10^{-6}$  ug/cm<sup>2</sup>/hr; the air concentration was  $7.515 \times 10^{-6}$  ug/m<sup>3</sup>.

## MATERIALS AND METHODS

Test Material(s): (s)-(E)-(p-chlorophenyl)-4,4-dimethyl-2-(1,2,4-triazol-1-yl)-1-penten-3-ol,  $^{14}\text{C}$ -labeled in the chlorophenyl ring, specific activity 27.1 Ci/mole, radiochemical purity 99.3%, optical purity >99%.

Soil: The soil used was a Muko sandy soil (characteristics shown in Table I). The soil was passed through a 2-mm sieve prior to use.

Test Formulation:

[REDACTED] were dissolved in 10 mL of methanol. One mL of the solution was evaporated (under reduced pressure) in a 30 mL pear-shaped flask. After evaporation of the solvent, 2.12 mL of distilled water were added, mixed well, and the resulting solution added to a solution of [ $^{14}\text{C}$ -Phenyl]-(S)-E-isomer (150 uCi, 1.615 mg) in 70 uL of cyclohexanone.

### Experimental Procedure:

- Soil Treatment - One mL of the test formulation was evenly (with a syringe) applied onto the soil (50 g on a dry-weight basis) contained in a 200 mL Erlenmeyer flask and mixed well to give a concentration of 15 mg ai/kg. The soil moisture was adjusted to 75% of field moisture by addition of the liquid formulation.
- Volatility studies - Figure 1 shows the equipment used in the studies, which were initiated immediately after the liquid formulation was applied. Moistened air (80+5%) passed over the treated soil at a controlled rate of 100 mL/min. The temperature of the system was maintained at  $25 \pm 1^\circ\text{C}$  throughout the experimental period. Any volatiles in the effluent air were trapped in a polyurethane foam plug. Both the test flask and the plug were wrapped with aluminum foil to prevent any photodegradation.

### Analytical Methods:

The extraction of volatile material trapped in the plugs was accomplished by washing the polyurethane foam three times with 25 mL of methanol. Aliquots (2 mL) of the combined eluates were radioassayed (in duplicate) by LSC. The low quantities of radioactivity made necessary that eluates sampled at 1-3, 4-9, and 11-30 days were concentrated by separately combining and evaporating to dryness under reduced

pressure; the residues were redissolved in a small volume of methanol.

After 30 days, soil samples were extracted with 150 mL of methanol/distilled water (25:5 by volume) followed by mechanical shaking (10 min). Soil and supernatant were separated by centrifugation (3000 rpm; 10 min; repeated three times). Combined extracts were concentrated under reduced pressure.

Extracts from the polyurethane foam plug and from the soil were analyzed by two-dimensional thin-layer chromatography (TLC) with solvents system A for the first direction and B for the second direction (Refer to Table II). Unextractable radioactivity in the soils was determined by LSC after combustion.

#### Calculations:

Volatilization rate (expressed as  $\mu\text{g}/\text{cm}^2/\text{hour}$ ) and air concentration of radioactivity (expressed as  $\mu\text{g}/\text{m}^3$ ) were calculated as follows:

$$(\text{Volatilization rate}) = \left( \frac{T}{2.22 \times 10^6} \right) \times \left( \frac{I}{R} \right) \times \left( \frac{I}{S} \right) \times [I / (24 \times d)]$$

$$(\text{Air Concentration}) = \left( \frac{T}{2.22 \times 10^6} \right) \times \left( \frac{I}{R} \right) \times [I / (F \times 60 \times 24 \times d)]$$

T = trapped radioactivity (in dpms)

R = specific radioactivity ( $92.9 \times 10^{-3} \text{ uCi}/\mu\text{g}$ )

S = surface area of the treated soil ( $60.8 \text{ cm}^2$ )

F = air flow rate (100 mL/min)

d = interval between samplings (in days)

#### REPORTED RESULTS

<sup>14</sup>C During the 30-day period, 0.012 - 0.014% of the applied <sup>14</sup>C was volatilized from the soil. At the end of the experiment, 100.4 - 100.3% of the initial dose remained in the soil. Extractable radioactivity in the soil was 92.3 - 92.6%, and nonextractable radioactivity was 7.4 - 7.6% of the dose. The main component in the soil extracts was the unchanged parent material (S)-E-isomer (90.9 - 91.5%), with a trace amount of the Z-isomer (<0.8%). The parent material was also a main component of the extracts of the polyurethane foam plug.

Volatilization rate and air concentration of radioactivity were maximal on the first day after treatment. The calculated volatilization rate was  $7.05 \times 10^{-3} \mu\text{g}/\text{cm}^2/\text{hour}$  and the air concentration was  $7.515 \times 10^{-2} \mu\text{g}/\text{m}^3$ ; both decreased gradually afterwards (Table II and Figure 2).

It was concluded that the volatilization rate of S-3307D (uniconazole) from soils is extremely slow and that the air concentration is extremely low.